Tuning Machine Learning Models for Prediction of Building Energy Loads

Abstract

There have been numerous simulation tools utilised for calculating building energy loads for the efficient design and retrofitting. However, these tools entail a great deal of computational cost and prior knowledge to work with. This issue is even further magnified, when making decisions for selecting building characteristics or retrofitting technologies, due to the required considerable number of calculations. One promising solution is utilising Machine Learning (ML) techniques which take the advantage of existing historical data for forecasting new samples and lead to informed decisions. This study investigates the accuracy of most popular ML models in the prediction of buildings heating and cooling loads, along with the newest techniques, carrying out specific tuning for each ML model. The results show that evaluating even a small sample of options for these choices can potentially deliver regression models that perform far better than the 'default' or most common options. They also indicate that ML models for each energy load should be tuned independently to obtain the best accuracy as input features affect them diversely. This concern is further elaborated using meta-model and global sensitivity analysis.

Keywords: Building energy loads, Energy prediction, Machine learning, Energy modelling, Energy simulation, Building design

1. Introduction

Buildings must be designed to maximise the health and well-being of their occupants while consuming the least energy and materials possible. Improving the building stock to achieve this goal requires improvements to existing buildings in addition to the new high-performance constructions. One approach to the design of high-performance buildings is performance-driven design, in which the energy demand to keep its occupants comfortable is approximated using a physics-based simulation program. This method is called Building performance Simulation (BPS), and it allows a designer/engineer to examine the influence of form, materials, and systems before construction on the expected thermal performance of a building. Conventionally, the search for an optimal design with simulation has been through a manual iterative process - design, analyse, change. This process is a labour-intensive task, so the search space, i.e., the space of possible options, is necessarily limited. The use of performance-driven design can, thus, be augmented with optimisation, since optimisation offers a way to expand the search boundaries during the design process significantly.

The benefits of optimisation over manual search are realised when the optimising routine is able to evaluate thousands of potential options (Si, 2017). However, large runs of performance simulations of realistic building models require significant time and computational resources. Optimisation reduces the specialist labour required to search very large spaces of options, but the resulting computational load can overwhelm the design process. The use of surrogate models has been proposed to overcome this problem (Zhao & Magoulès, 2012a; Yu et al., 2016; Rastogi et al., 2017; Seyedzadeh et al., 2018). Surrogate models, or emulators, are mathematical relationships between inputs and outputs of interest from the system being studied, learnt from measured or simulated data that represents the physical problem. For example, the thermo-physical properties of building materials and weather parameters can be used to predict indoor environmental conditions, as we do in this paper. Sufficiently accurate surrogate models especially Machine Learning (ML) methods, thus, provide fast and accurate alternatives to building performance simulators during a computationally-intensive design process (Rastogi et al., 2017).

The use of surrogate models requires careful consideration of the accuracy and appropriateness of the data and relationships inferred from the data. In this paper, we examine a practical aspect of this approach: selecting and tuning regression models. By this, we mean selecting the model types, structures, and parameters most appropriate to the problem at hand. We show that the process of choosing a model must account not just for predictive accuracy but also model complexity, ease of use, and consistency of predictions. We use the datasets described in Tsanas & Xifara (2012); Rastogi (2016) to demonstrate the performance of different candidate models. Besides, the application of ML in evaluating the importance of the input variables in calculation of heating and cooling loads is presented. We end with a discussion of how these techniques may be used in a computationally-intensive design process.

The paper is organised as follows. The next section presents a review of previous studies and issues with using ML models in predicting building energy consumption. That is followed by the methods, description of the case studies, and results. The final section contains recommendations on model selection and discusses future work.

2. Background and Motivation

Machine Learning refers to a set of algorithms that can learn from existing data (inputs and outputs) to predict outputs on new, unseen inputs. The learning algorithms are divided into two categories: supervised learning, in which the target is known, and unsupervised learning, where there is no "output" to learn and predict. A supervised learning is either one of regression or classification, in which input features (X) are mapped to one or more output variables (Y). Unsupervised learning includes techniques such as clustering, which organises data into groups based on similarities among the samples in a dataset. Unsupervised learning is applied to an unlabelled dataset, i.e., where the there are no labels to test against, while a supervised learning algorithm detects the relation between inputs and output and used this function to predict new records.

The use of machine learning models in the analysis of buildings was first used by Kalogirou et al. (1997) to estimate building heating loads considering envelope characteristic along with the desired temperature. The work was completed in 2000 by using ANN to predict the hourly energy demand of holiday dwellings, calculated using ZID software. Kalogirou et al. (2001) also used ANN to estimate the daily heat loads of model house buildings with different combinations of the wall and roof types (i.e. single vs. cavity walls and roofs with different insulation applied) using a typical meteorological data for Cyprus. In that study, TRNSYS was used to estimate energy use and the data validated by comparison of one building energy consumption with the actual measurement.

A global optimisation method coupled with the ANN was used to predict cooling load demand (Yokoyama et al., 2009). In this research, authors probed two parameters of the network namely number of hidden layers and neurons in each of them. Paudel et al. (2014) incorporated occupancy profile as well as operational heating power level features with climate variables to model the heating energy consumption using ANN. In order to increase the accuracy of the prediction model time dependant attributes of operational heating power level was further included. Later in 2016, Deb et al. (2016) employed five previous day's data as ANN model inputs to forecast daily cooling demand of three institutional buildings in Singapore.

Mena et al. (2014) applied ANN for short-term forecasting of hourly electricity consumption. A large time series covering two years was collected from a solar centre in Spain.The outcome was highlighting high impact of outdoor temperature and solar radiation on electricity usage. Principal component analysis (PCA) was employed by Platon et al. (2015) to explore feature selection of ANN model in the prediction of hourly electricity consumption of an institutional building. In another work, Li et al. (2015) used PCA fro reducing input variables space. Furthermore, they introduced a new optimisation algorithm to improve performance of the utilised ANN model in short-time forecasting of electricity demand.

Neto & Fiorelli (2008) applied ANN for daily prediction of a commercial building daily energy usage and demonstrated that in supervised learning produce more accurate outputs comparing with EnergyPlus software. Besides, improper assessment of lighting and occupancy was recognised as the main source of model uncertainty. For that reason, Dombayci (2010) employed degree-hour method to deduce the hourly energy demand to be used in ANN training. The performance of proposed approach is accurate provided that only few building characteristic is taken into account. Hence, the model is most appropriate for single single building energy management of simple residential buildings.

Yalcintas (2006) applied ANN to approximate the energy performance of sixty educational building stock located in Hawaii. The training data collected from previous energy assessments reports considering building general and air conditioning system characteristics. Wong et al. (2010) estimate the dynamic energy performance of a commercial building with day-lighting. Building daily energy usage was calculated using EnergyPlus coupled with an algorithm for deriving the interior reflection and used in ANN model. It was revealed by Hong et al. (2014b) that comparing to statistical analysis, ANNs are more accurate in evaluating energy performance of schools in the UK. To that end, Khayatian et al. (2016) applied ANN to predict energy performance certificates of domestic buildings in Italy. Ascione et al. (2017) investigated the association of energy usage and occupant thermal comfort in predication of energy performance. The energy consumption was calculated using EnergyPlus, and the records are fed to ANN model which is then used as the main engine for optimisation of new building design and retrofit planning.

SVM for building energy forecasting was introduced by Dong et al. (2005) in 2005. The model was trained over a dataset in which temperature, humidity and solar radiation considered as the features. The short-time prediction of electricity consumption using SVM was further investigated by Li et al. (2009a) and Massana et al. (2015). In an other Li et al. (2009b) and Hou & Lian (2009)utilised SVM to forecast hourly cooling leads of an office building considering the same parameters suggested by Dong et al. (2005). Xuemei et al. (2009) improved the performance of SVM used for predicting cooling loads by contributing to learning correction for limited training sets and enhanced prediction time efficiency to traditional SVM model in load forecasting. Later Li et al. (2010) applied SVM for yearly estimation of electricity consumption in domestic buildings. The model considered building envelope parameters as well as the annual electricity consumption normalised by unit area. Aiming at optimising new office building design, Zhao & Magoulès (2010) applied a parallel implementation of SVM to calculate energy usage. The work was improved by reducing input variable space through applying gradient guided feature selection and the correlation coefficients methods. Jain et al. (2014) investigated the impact of different time interval and building spaces in data collection one energy demand forecasting using SVM. (Chen & Tan, 2017) used and SVM model coupled with multi-resolution wavelet decomposition for estimating energy consumption of various building type.

Since early 2000, GP regression has been employed by researchers in different application especially where there are uncertainties in input parameters (Jiang et al., 2010; Grosicki et al., 2005; Bukkapatnam & Cheng, 2010). In building energy modelling, there are usually uncertainties in the section of appropriate values for some characteristics (e.g. envelope insulation). Heo et al. (2012); Heo & Zavala (2012) utilised GP modelling to estimate to uncertainty levels in calculating building energy saving after retrofitting. For the same purpose, Zhang et al. (2013) applied GP for predicting the post-retrofit phase energy demand of an office building. Burkhart et al. (2014) incorporated GP with a Monte Carlo expectation maximisation algorithm to train the model under data uncertainty, aiming at optimisation of office building HVAC system performance. It was revealed that the models can be trained even with limited data or sparse measurements employing rough approximation and data range instead of sensor data. Rastogi et al. (2017) compared the accuracy of GP and linear regression in emulating of a building performance simulation and show that the accuracy of GP is four times better than linear regression testing on EnergyPlus simulated case studies located in the US.

Ensemble ML models such as Random Forest (RF) and Gradient Boosted Regression Trees (GBRT) have been introduced for decades, the use of them in building energy domain is very new. Tsanas & Xifara (2012) applied RF for estimating energy consumption using building characteristics. They compared the results with the iteratively reweighted least squares method, and showed that the ML model outweighed in term of accuracy. Papadopoulos et al. (2017) compared tree-based models in building energy performance estimation using the data provided by Tsanas & Xifara (2012). Lately, Wang et al. (2018) used RF for short-time prediction of energy usage in an office building considering compound variables of envelope, climate and time.

Several studies presented a comparison between the performance (accuracy) of main utilised ML model and one/few other ML model(s) or generally basic models such as MLR. ANN was used for energy performance estimation in commercial buildings, comparing the accuracy of MLR (Yalcintas & Ozturk, 2007; Yalcintas, 2006) and engineering models Hong et al. (2014a). Platon et al. Platon2015a compared ANN with case-based reasoning (CBR) for prediction of hourly electricity consumption of an institutional building. Li et al. (2009b) applied SVM to forecast hourly cooling loads of an office building and provided a comparison with ANN indicating that SVM and general regression ANN had more potential for being used in the field of building energy. Edwards et al. Edwards et al. (2012) also evaluated the accuracy of SVM and ANN in forecasting hourly energy consumption of residential buildings and found ANN as the least accurate model. Rastogi et al. (2017) compared the accuracy of GP and linear regression in emulating an EnergyPlus building performance simulation based on case studies in U.S.A and ascertained that the accuracy of GP is far better than linear regression. Manfren et al. (2013) used GP with RFB kernel and MLR to predict monthly electricity and gas usage of heating and cooling systems signifying the supremacy of the ML model. Zhang et al. (2015) compared change point, Gaussian-based and one layer ANN models for prediction of an office buildings hot water energy consumptions and concluded that ANN models can be inefficient when enough data is not fed through the system. Tsanas & Xifara (2012) investigated the accuracy of RF and iteratively re-weighted least squares regression model. Wang et al. (2018) indicated the superiority of RF over SVM and regression trees in predicting hourly building energy demands.

Most of these studies considered either a comparison between conventional (or simple) ML models such as one layer ANN or only optimised a limited part of a model. Whereas, model hyper-parameters are assumed driving forced to govern the learning processes, especially when using a complex model with a high number of parameters such as ANN. On the other hand, accuracy of models with a set of optimised pre-identified parameters can vary from one dataset to another. With these considerations, the previous works do not provide a fair evaluation of different models and the decision making about model selection for similar building energy datasets can become a very difficult task.

This research addresses the aforesaid issues by evaluating the accuracy of the ML models over two different well-established building datasets, and carefully tuning hyper-parameter of each model. The aim was to predict heating and cooling loads of buildings accurately, i.e. to create a fast and reliable model as an alternative for BPS tool. The work contributes to building energy forecasting, which is an essential gateway for energy efficient design and optimal retrofitting.

3. Machine Learning Models

ML models operate as a black box, so further information about the building is not required. The general scheme of supervised learning for modelling building energy is illustrated in Figure 1. As seen, the first step is to select a set of features for representing the building energy system. Although data-driven methods build models with fewer variables than engineering techniques, it is crucial to generate a logical input set for ML model. These features are not necessarily raw building characteristics or weather data; instead they could be complex variables calculated from basic ones, e.g. wall to floor ratio and mean daily global radiation (Zhao & Magoulès, 2012b).

The next key stage in utilising MLs is optimisation of model itself. This procedure which is called tuning plays an important role in performance of a ML model especially when it is a complex one. Choosing inappropriate hyper-parameters will results in poor accuracy which may falsely be translated as the model failure. Although selecting the right input variables is essential for

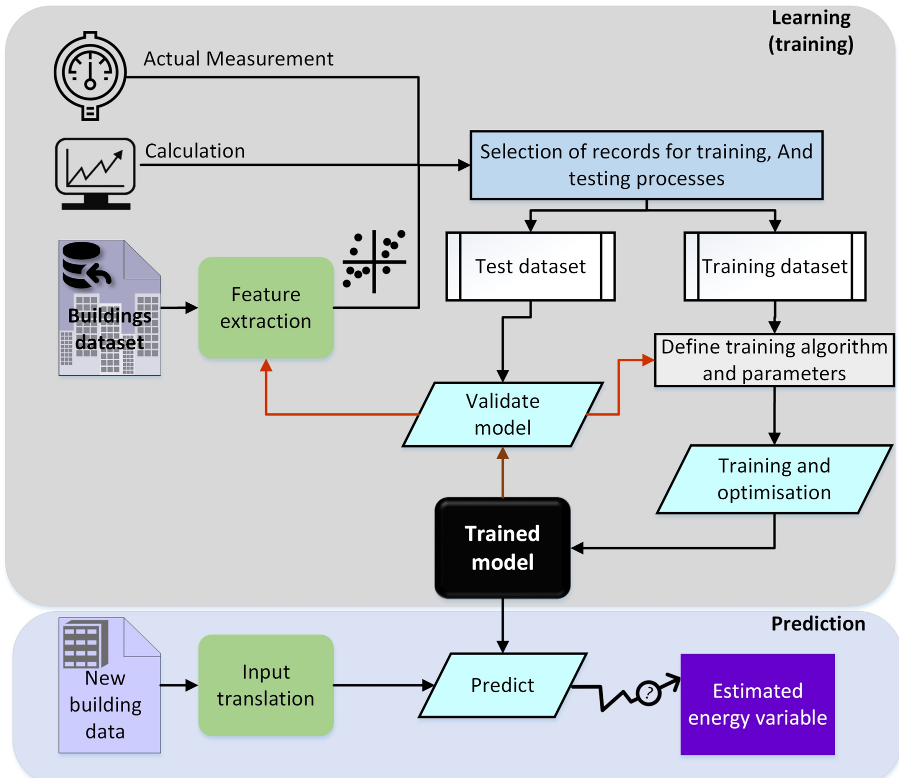


Figure 1: General schematic diagram of supervised learning.

training a successful machine, the full advantage cannot be taken of ML without tuning the model for that specific training data. Each ML has different hyper-parameters which govern the learning process. A key point in tuning a ML model parameters is the generalisation. That is to say the how well the learning model applies to specific examples not seen by the model when it was training. Hence, in the procedure of model optimisation there should be a good mechanism such as cross-validation in order to avoid overfitting (i.e. modelling the training data too well).

Five ML techniques including ANN, SVM, GP, RF and GBRT are employed to emulate two BPS tools namely EnergyPlus and Ecotect. Hyper-parameters are tuned by a grid-search procedure using 10-fold cross-validation on the training dataset. Furthermore, different normalisations such as standard, min-max and robust are applied to data before training procedure. Robust scaler eliminates the median and normalises data according to the inter-quartile range.

Basics of each model and the parameters going under optimisation are explained as followings.

3.1. Artificial Neural Network

Neural networks have been broadly utilised for building energy estimation and known as the major ML techniques in this area. They have been successfully used for modelling non-linear problems and complex systems. By applying different techniques, ANNs have the capability to be immune to the fault and noise (Tso & Yau, 2007) while learning key patterns of building systems.

The main idea of ANN is obtained from the neurobiological field. Several kinds of ANN have been proposed for different applications including, Feed Forward Network (FFN), Radial Basis Function Network (RBFN) and recurrent networks (RNN). Each ANN consists of multi-layers (minimum two layers) of neurons and activation functions that form the connections between neurons. Some frequently used functions are linear, sigmoid ad hard limit functions (Park & Lek, 2016).

In FFN which was the first NN model as well as the simplest one, there are no cycles from input to output neurons and the pieces of information moves in one direction in the network. Figure 2 illustrates the general structure of FFN with input, output and one hidden layer.

RNN uses its internal memory to learn from preceding experiences by allowing loops from output to input nodes. RNN is proposed in various architectures including fully connected, recursive, long short-term memory, etc. This type of neural network has usually been employed to solve very deep learning tasks such as multivariate time-series prognostication; often more than 1000 layers are needed (Ghiassi et al., 2005).

In RBFM, a radial basic function is used as activation function providing a linear combination of inputs and neuron parameters as output. This type of

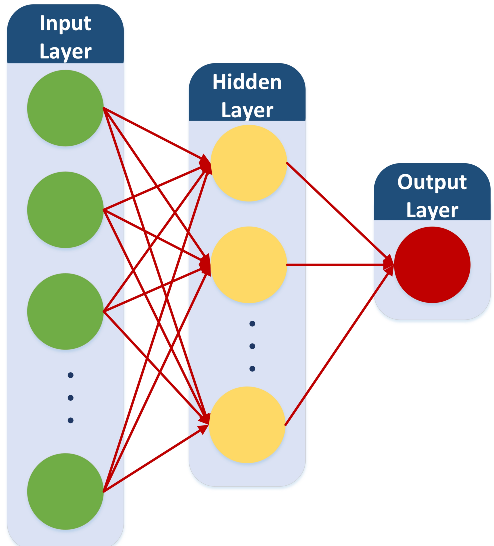


Figure 2: Conceptual structure of feed forward neural network with three layers.

network is very effective for time series estimation (Harpham & Dawson, 2006; Leung et al., 2001; Park et al., 1998).

Due to the nature of the datasets, a multilayer perception FFN is utilised in this work. The ANN hyper-parameters which go under optimisation are:

- **Optimiser:** the function that updates the weights and bias;
- **Activation:** a non-linear transformation function which is applied over the input, and then the output is fed to the subsequent layer neurons as input. An ANN without activation function will act as a linear regressor and may fail to model complex systems;
- **Initialisation:** the initial values of weights before the optimiser is applied for training;
- **Epoch:** the number of forward and backward passes for all samples of data;
- **Batch size:** specifies the number of samples that are propagated through

the ANN training (i.e. the number of samples in one epoch);

- **Dropout rate:** dropout is a regularisation method for preventing ANN from overfitting and creating more generalised model by randomly rejecting some neurons during training. Droput rate determines the percentage of randomly input exclusion at each layer;

- **Size:** number of neurons in each layer and number of layers.

3.2. Support Vector Machine

SVMs are highly robust models for solving non-linear problems and used in research and industry for regression and classification purposes. As SVMs can be trained with few numbers of data samples, they could be right solutions for modelling study cases with no recorded historical data. Furthermore, SVMs are based on the Structural Risk Minimisation (SRM) principle that seeks to minimise an upper bound of generalisation error consisting of the sum of training error and a confidence level. SVMs with kernel function acts as a two-layer ANN, but the number of hyper-parameters is fewer than that. Another advantage of SVM over other ML models is uniqueness and globally optimality of the generated solution, as it does not require non-linear optimisation with the risk of sucking in a local minimum limit. One main drawback of SVM is the computation time, which has the order almost equal to the cube of problem samples.

Suppose every input parameter comprises a vector X_i (i denotes the ith input component sample), and a corresponding output vector Y_i that can be building heating loads, rating or energy consumption. SVM relates inputs to output parameters using the following equation:

$$Y = W \cdot \phi(X) + b \tag{1}$$

where $\phi(X)$ function non-linearly maps X to a higher dimensional feature space. The bias, b, is dependent of selected kernel function (e.g. b can be equal to zero for Gaussian RBF). W is the weight vector and approximated by empirical risk function as:

$$Minimise: \frac{1}{2}\|W\|^2 + C\frac{1}{1}\sum_{i=1}^{N} L_\varepsilon(Y_i, f(X_i)) \tag{2}$$

L_ε is ε-intensity loss function and defined as

$$L_\varepsilon(Y_i, f(X_i)) = \begin{cases} |f(x) - Y_i| - \varepsilon, & |f(x) - Y_i| \geq \varepsilon \\ 0, & otherwise \end{cases} \tag{3}$$

Here ε denotes the domain of ε-insensitivity and N is the number of training samples. The loss becomes zero when the predicted value drops within the band area and gets the difference value between the predicted and radius ε of the domain, in case the expected point falls out of that region. The regularised constant C presents the error penalty, which is defined by the user.

SVM rejects the training samples with errors less than the predetermined ε. By acquisition slack variables ξ and ξ_i^* for calculation of the distance from the band are, equation (3) can be expressed as:

$$\underset{\xi,\xi_i^*,W,b}{Minmise}: \frac{1}{2}\|W\|^2 + C\frac{1}{N}\sum_{i=1}^{N} \xi + \xi_i^* \tag{4}$$

subject to

$$\begin{cases} Y_i - W \cdot \phi(x_i) - b \leq \varepsilon + \xi \\ W \cdot \phi(x_i) + b - Y_i \leq \varepsilon + \xi_i^* \\ \xi \geq 0, \quad \xi_i^* \geq 0 \end{cases} \tag{5}$$

The SVM problem using a kernel function of $K(X_i, X_j)$ (α_i, α_i^* as Lagrange multipliers) can be simplified as:

$$\underset{\{\alpha_i\},\{\alpha_i^*\}}{Maximise}: -\varepsilon\sum_{i=1}^{N}(\alpha_i^* + \alpha_i) + \sum_{i=1}^{N} Y_i(\alpha_i^* - \alpha_i) - \\ \frac{1}{2} sum_{i=1}^{N} \sum_{j=1}^{N}(\alpha_i^* - \alpha_i)(\alpha_j^* - \alpha_j)K(X_i, X_j) \tag{6}$$

subject to

$$\sum_{i=1}^{N}(\alpha_i^* - \alpha_i) = 0, \qquad 0 \leq \alpha_i, \alpha_i^* \geq C \tag{7}$$

As mentioned before the number of parameters in SVM with a Gaussian RBF kernel is few as two which are C and Gamma.

3.3. Gaussian Process

The main drawback of GP modelling is expensive computational cost, especially with the increase of training samples. This is due to the fact that GP constructs a model by determining the structure of a covariance matrix composed of $N \times N$ input variable where the matrix inversion required in predictions has a complexity of $O(N^3)$

Given a set of n independent input vector X_j $(j = 1, \cdots, n)$, the corresponding observations of y_i $(i = 1, \cdots, n)$ are correlated using covariance function K with normal distribution equal to (Li et al., 2014):

$$P(y; m; k) = \frac{1}{(2\pi)^{n/2}|K(X,X)|^{1/2}} \times exp\left(-\frac{1}{2}(y-m)^T K(X,X)^{-1}(y-m)\right) \tag{8}$$

The covariance or kernel function can be derived as

$$K = \begin{vmatrix} k(x_1,x_1) & k(x_1,x_2) & \cdots & k(x_1,x_n) \\ k(x_2,x_1) & k(x_2,x_2) & \cdots & k(x_2,x_n) \\ \vdots & \vdots & \ddots & \vdots \\ k(x_n,x_1) & k(x_n,x_2) & \cdots & k(x_n,x_n) \end{vmatrix} \tag{9}$$

A white noise, σ, is presumed in order to consider the uncertainty. It is assumed that the samples are corrupted (lets suppose as new inputs as x^*) by this noise. In this case covariance of y is expressed as

$$cov(y) = K(X,X) + \sigma^2 \tag{10}$$

Then y^* can be estimated as below.

$$y^* = \sum_{i=1}^{n} \alpha_i k(x_i, x^*) \tag{11}$$

$$\alpha_i = \left(K(X,X) + \sigma^2 I\right)^{-1} y_i \tag{12}$$

For GP model three parameters are tuned: kernel, alpha (α) which is the value added to the diagonal of the kernel matrix (equation 11) and the number of restarts of the optimiser for discovering the parameters maximising the log-marginal probability. Two combinations of white noise with RBF and Matern covariance functions are used for GP model kernel. Matern kernel is denied as:

$$K(X,X') = \frac{261-v}{\Gamma(v)} \left(\frac{\sqrt{2v} \mid x - x' \mid}{I} \right)^{v} K_v \left(\frac{\sqrt{2v} \mid x - x' \mid}{I} \right) \tag{13}$$

Here, Γ is the Gamma function and K_v is the modified Bessel function the second-order v (Owen et al., 1965).

3.4. Random Forest

Random forest is a collection (ensemble) of randomised decision trees (DTs) (Tin Kam Ho, 1995). DT is a non-parametric ML that establishes a model in the form of a tree structure. DT repeatedly divides the given records into smaller and smaller subsets until only one record remains in the subset. The inner and final sets are known as nodes and leaf nodes. As the precision of DT is substantially subject to the distribution of records on in the learning dataset, it is considered as an unstable method (i.e. tiny alteration in the observations will change the entire structure). To overcome this issue a set of DTs and uses the average predicted values of all independent trees as the final target. In general, RF applies bagging and boosting to combine separate models but with sore of similar information and generate a linear combination from many independent trees.

RF requires few number of hyper-parameters to be set. The main parameter is the number of independent trees in the forest. There is a trade-off between the accuracy of model and training/prediction computational cost. Thereby, this parameter should be tuned to choose the optimal value. Other parameters include the number of features to consider when seeking for the best split, whether bootstrap samples are used when creating trees and minimum number of data sample to split a node and required in each node.

3.5. Gradient Boosted Regression Trees

Like RF, GBRT is an ensemble of other prediction models such as DTs. The principal difference between GBRT and RF is that the latter one is based on fully developed DTs with low bias and high variance, while the former employs weak learners (small trees) having high bias and low variance (Breiman, 2017). In GBRT, trees are not independent of each other; instead, each branch is created based on former simple models through a weighting procedure. At each inner node (i.e. the split point) given dataset is divided into two samples. Let's assume a GBRT with three nodes trees; then there will be one split point in which the best segmentation of the data is decided, and the divergence of the obtained values (from the individual averages) are calculated. By fitting on these residuals, the subsequent DT will seek for another division of data to reduce the error variance.

Most important parameters for optimising GBRT comprise learning rate (also known as shrinkage) which is a weighting procedure to prevent overfitting by controlling the contribution of each tree, number of trees, maximum depth of tree and the number of features for searching best division, and minimum number of data sample to split a node and required in each node. Moreover, sub-sample parameter defines the fraction of observation to be selected for each tree.

Rather than conventional GBRT model the recently improved version known as eXtreme Gradient Boosting (XGBoost) algorithm (Chen & Guestrin, 2016) is also evaluated with similar parameters, but some differences. The minimum sum of instance weight controls the generalisation similar to minimum sample split in GBRT. The portion of columns when constructing each tree (colsample bytree) similar to maximum features.

3.6. Performance Evaluation

Various measurements based on actual and predicted results are calculated, in order to evaluate the performance or accuracy of data-driven models. These include Coefficient of Variance (CV), Mean Bias Error (MBE), Mean Squared Error (MSE), Root Mean Squared Error (RMSE), Mean Squared Percentage error (MSPE), Mean Absolute Percentage Error (MAPE) and MAE (mean absolute error). CV is the variation of overall prediction error concerning actual mean values. MBE is used to determine the amount over/underestimation of predictions. MSE and MSPE is a good inductor of estimation quality. MAE determines the average value of the errors in a set of forecasts and MAPE is the percentage of error per prediction. RMSE has the same unit of actual measurements. In this work, RMSE, MAE and **coefficient of determination** (R^2) are used to present the accuracy of ML models. R^2 is the percentage variance in the dependent variable explained by the independent ones. These values are calculated as follows:

$$RMSE = \sqrt{\frac{1}{N}\sum(y_i - \hat{y})^2} \tag{14}$$

$$MAE = \frac{1}{N}\sum \mid y_i - \hat{y} \mid \tag{15}$$

$$R^2 = \frac{\sum(\hat{y}_i - \bar{y})^2}{\sum(y_i - \bar{y})^2} \tag{16}$$

Here, y, $\hat{y}$ and $\bar{y}$ represent the real, estimated and average response values, respectively.

4. Selected Datasets for Case Study

Two building datasets simulated using BPS tools are utilised. First data contains 768 variations of a residential building obtained altering eight basic envelope characteristic (Tsanas & Xifara, 2012), and the second dataset includes various building type represented by 28 envelope and climate features (Rastogi, 2016). Each set and the distribution of variables are presented in this section. The prediction targets for both sets are heating and cooling loads.

4.1. Ecotect Dataset

This dataset was developed for the research work by Tsanas & Xifara (2012) and obtained from UCI machine learning repository (Xifara & Tsanas, 2012). The worked studied 12 residential buildings types all sharing the same volume equal to $771.75m^3$ and also the same characteristics except the ones provided in Table 1. The choice of material was based on the availability in the construction market. The materials are selected in a way to have lowest U-Values (walls: 1.78, floors: 0.86, roofs: 0.50 and windows: 2.26). The values for orientation are numerically coded as following: 2 for North, 3 as East, 4 representing South and 5 for West. The glazing area (percentage of glazing to floor area) is assigned with four values from 0% to 40%. The glazing distribution in each faade of the building has 6 variations as: (0) uniform; with 25% glazing on each side, (1) 55% glazing on the north faade and 15% on the rest, (2) 55% glazing on the east faade and 15% on the rest, (3) 55% glazing on the south faade and 15% on the rest, (4) 55% glazing on the west faade and 15% on the rest, and (5) no glazing. All the combinations of input parameters the heating and cooling loads are simulated using Ecotect tool in which buildings are assumed to be in Athens city and be occupied by seven people with sedentary activity. A mixed mode with 95% efficiency and thermostat range of 19-24$°C$ was presumed for the thermal properties. The operating hours were set to 15-20 for weekdays and 10-15 h for weekends. The lighting level was set to 300 lx.

Figure 3 illustrates the frequency of features as histogram graphs. The correlation between each pair of input and target variables is demonstrated using heatmap matrix in Figure 4.

Table 1: List of features that represent the characteristics of residential buildings for prediction of energy loads

Feature	Unit	Range	Variation	Code
Inputs				
Relative compactness	-	0.62 – 0.98	12	rc
Surface area	m^2	514 – 808	12	sa
Wall area	m^2	245 – 416	7	wa
Roof area	m^2	110 – 220	4	ra
Overall height	m	3.5, 7	2	oh
Orientation	-	2 – 5	4	ori
Glazing area	m^2	0 – 0.4	4	glza
Glazing area distribution		0 – 5	6	glzd
Targets				
Heating load	KWh/m^2	6 – 43	-	heat
Cooling load	KWh/m^2	10 – 48	-	cool

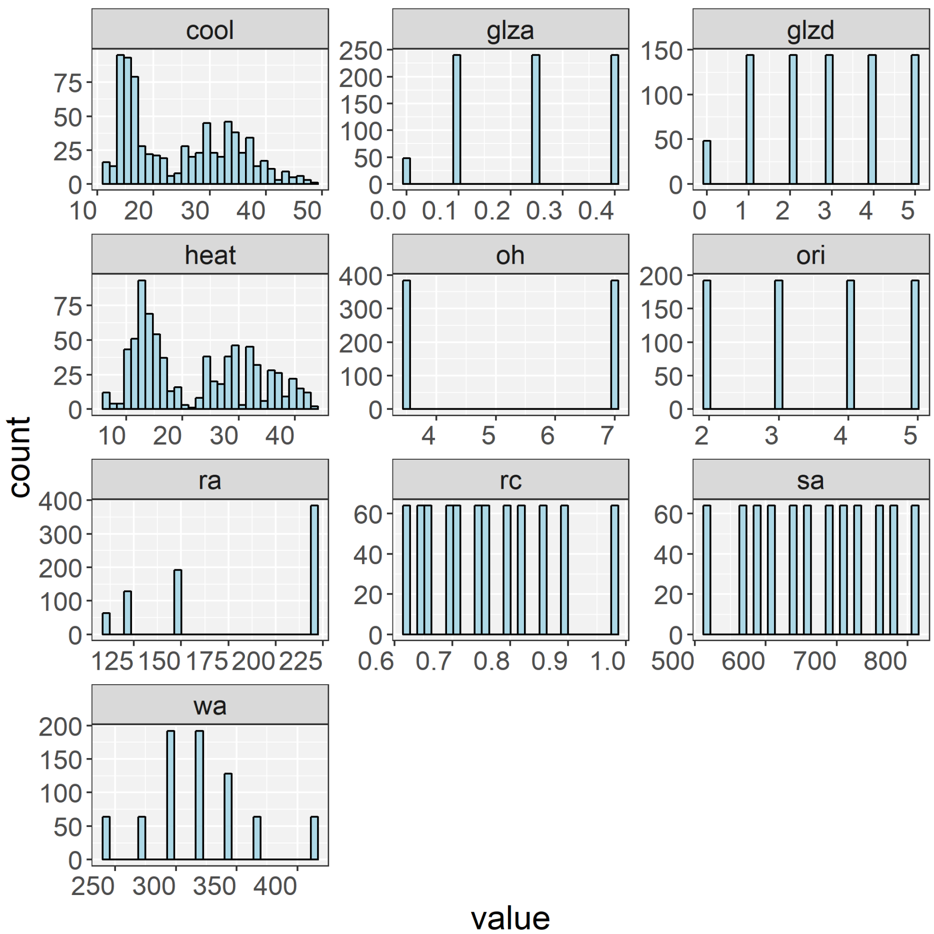


Figure 3: Distribution of features for Ecotect data.

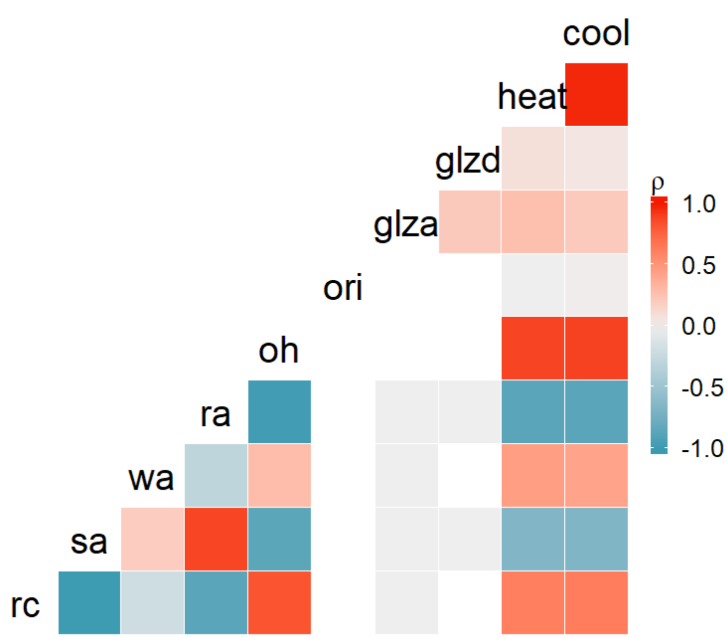


Figure 4: Ecotect data features correlation map.

4.2. EnergyPlus Dataset

This datasets consists of two commercial and residential databases. The former dataset was originally acquired from the US Department of Energy (US-DOE) commercial reference building models published at 2011 and processed by Rastogi (2016). The US-DOE set considered sixteen types and sub-blocks of buildings classified into eight overall groups based on usage. Table 2 presents the building types which are considered in the simulations and the frequency of each with unique features. For each subtype there are three variations for envelope construction: pe-1980, post-1980, and new construction, however all have the same building form, area and operation schedules. The reference building models as EnergyPlus input files can be obtained freely from (DOE). Rather than US-DOE data, a single-family home case is included in simulation dataset which is example of a simple study. The aim of the latter data was to provide a case which can be modelled using simple regression for the sake of comparison. Finally, extra variation of US-DOE building models using synthetic weather data enabling calculation of the uncertainty in building simulation due to weather inputs (Rastogi, 2016). The climate data consists both real information recorded in different cities all around the world and generated synthetic weather data (Rastogi & Andersen, 2015). In total The dataset includes 460,000 buildings simulations characterised by 7 structural, 16 climate and 3 mixed features as presented in Table 3.

The feature selection was based on correlation estimation and PCA. The climate variables was derived from weather file provided for each region or city. These features are extracted from typical meteorological year, short-time records or the generated synthetic weather files and independent of buildings which are simulated. The building features are related to physical characteristics of the building envelope. These inputs was chosen on the basis of impact on the heating and cooling loads and calculated from geometry, material and structure properties. The mixed parameters represent the interactions between weather and buildings. Finally, the internal heat gain which is indispensable factor in characterising thermal simulation and considered as the user input was also

Table 2: Frequency and size of building types in EnergyPlus data

Building Usage	Type	Area (m^2)	Volume (m^3)	No. of E+ zones	No. of samples
Health	Hospital	22,422	88,864	55	3827
	Outpatient	3,804	11,932	118	5504
Home	Mid-rise Apartment	3,135	9,553	36	37173
	Single Family	78532			
Hotel	Large	11,345	35,185	43	5504
	Small	4,014	11,622	67	5468
Office	Large	46,320	178,146	73	275345
	Medium	5503	4,982	18	19,741
	Small	511	1,559	5	5483
Restaurant	Full Service	5,502	55,035	2	3824
	Quick Service	232	708	2	5505
Retail	Stand Alone	2,294	13,993	5	5503
	Strip_Mall	2,090	10,831	10	5498
	Supermarket	45,002	900,272	6	5554
School	Primary	6,871	27,484	25	5505
	Secondary	19,592	95,216	46	5507
Warehouse	–	4,835	39,241	3	5492

included in the dataset.

Table 3: List of EnrgyPlus features extracted for model training

Group	QTY	Stats	Description	Range	Code	Unit
Building	U-value	Average	Average U-value of envelope	0.14–6.06	*uval*	W/m^2K
	Thermal Mass	Sum	Sum of thermal storage capacity	1e-4–7.61	*tmass*	MWh/K
	Envelope Ratios	Ratio	Ratio of window area to wall area	0.58–85.00	*wwr*	-
			Ratio of window area to floor area	0.01–0.42	*wfr*	-
	Massing	Ratio	Form Factor (Volume / Wall Area)	2.47–17.14	*ff*	-
			Roof Ratio (Roof / Wall Area)	0.31–2.73	*rr*	-
Mixed	Shading	Average	Average sunlit percentage of envelope	0.35–100	*avgsunperc*	%
	Infiltration	Sum	Annual sum of energy gained due to infiltration	0–0.74	*suminfgain*	GWh
			Annual sum of energy lost due to infiltration	-2.7– -1e-4	*suminfloss*	
Other		Sum	Annual sum of Internal Heat Gain	0.03–5.24	*sumIHG*	GWh

Figure 5 illustrates the frequency of features as histogram graphs for Ener-

List of features extracted for model training (cont.)

GRP	QTY	Stats	Name	Range	Code	Unit
Climate	Degree Days	Sum	Annual sum of cooling degree days	(9.6–160)e4	*cdd*	*C-day*
			Annual sum of heating degree days	424–64878	*hdd*	
	Dry Bulb Temp (Hourly)	Avg.	Annual average of dry bulb temperature	-3.11–28.39	*avgtdb*	*C*
		Median	Median dry bulb temperature	-7.20–30	*medtdb*	
		IQR	Inter-quartile range of dry bulb Temp	3.6–34	*iqrtdb*	
	Dry Point Temp (Hourly)	Avg.	Annual average of dry point temperature	-7.41–21.43	*avgtdp*	*C*
		Median	Median dew point temperature	-6.4–24.2	*medtdp*	
		IQR	Inter-quartile range of dew point temperature	0–26.8	*iqrtdp*	
	Global Horizontal Irradiation (Hourly)	Avg.	Annual average of global horizontal irradiation	190–509	*avghi*	*MWh/m2*
		Sum	Annual sum of global horizontal irradiation	0.40–2.23	*sumghi*	
		IQR	Inter-quartile range of global horizontal irradiation	(0.84–5.2)e-3	*iqrghi*	
	Direct Normal Irradiation (Hourly)	Avg.	Annual average of direct normal irradiation	57–676	*avgdni*	*MWh/m2*
		Sum	Annual sum of direct normal irradiation	-10.34–3.15	*sumdni*	
		IQR	Inter-quartile range of direct normal irradiation	(0.38–26.3)e-4	*iqrdni*	
	Humidity (Hourly)	Avg.	Annual average of relative humidity	22–98	*avrh*	%
		Median	Median relative humidity	18–99.6	*medrh*	

gyPlus Dataset. It can be seen that the each variable is relatively distributed over the possible predefined values. The correlation heat-map matrix presented in Figure 6 shows the in dependency of different features especially building physics related ones from each other.

5. Result and Discussions

All models are implemented using Python programming language and test have been carried out on a PC with Intel Core i7-6700 3.4GHz CPU, 32GB RAM.

First, different models are tuned for estimating heating and cooling loads of building simulated by Ecotect. To test the accuracy of the ML model, k-fold cross-validation is used. The result is represented in Table 5 as R^2, RMSE and MAE for evaluating models accuracy and training and prediction time with the best combination of hyper-parameters, average fitting time of all tested models and the total number of iterations for comparison of time complexity. Here, the test time is the average of predictions of all folds for 192 samples.

In order to highlight the importance of tuning ML model for building energy data, it is worth to compare the result obtained from this study with the original work which used a default RF (Tsanas & Xifara, 2012). This paper reported RMSE of 1.014 and 2.567 for heating and cooling loads, respectively. Our best RF model achieved 0.476 and 1.585 for the same variants indicating minimum 40% improvement in accuracy. As discussed earlier, this data contains a simple structure, and most ML techniques deliver high accuracies. Hence, the precise model tuning becomes more essential when the studied building sets become more complicated.

It can be seen that the lowest RMSE for both heating and cooling loads is achieved by XGBoost, then GBT and RF. These models are all based on decision trees, but unlike RF the other two does not build independent trees. Hence, they train models slightly faster than RF. Considering accuracy and prediction time, GBT seems to be most desired method for this specific dataset. However, NN

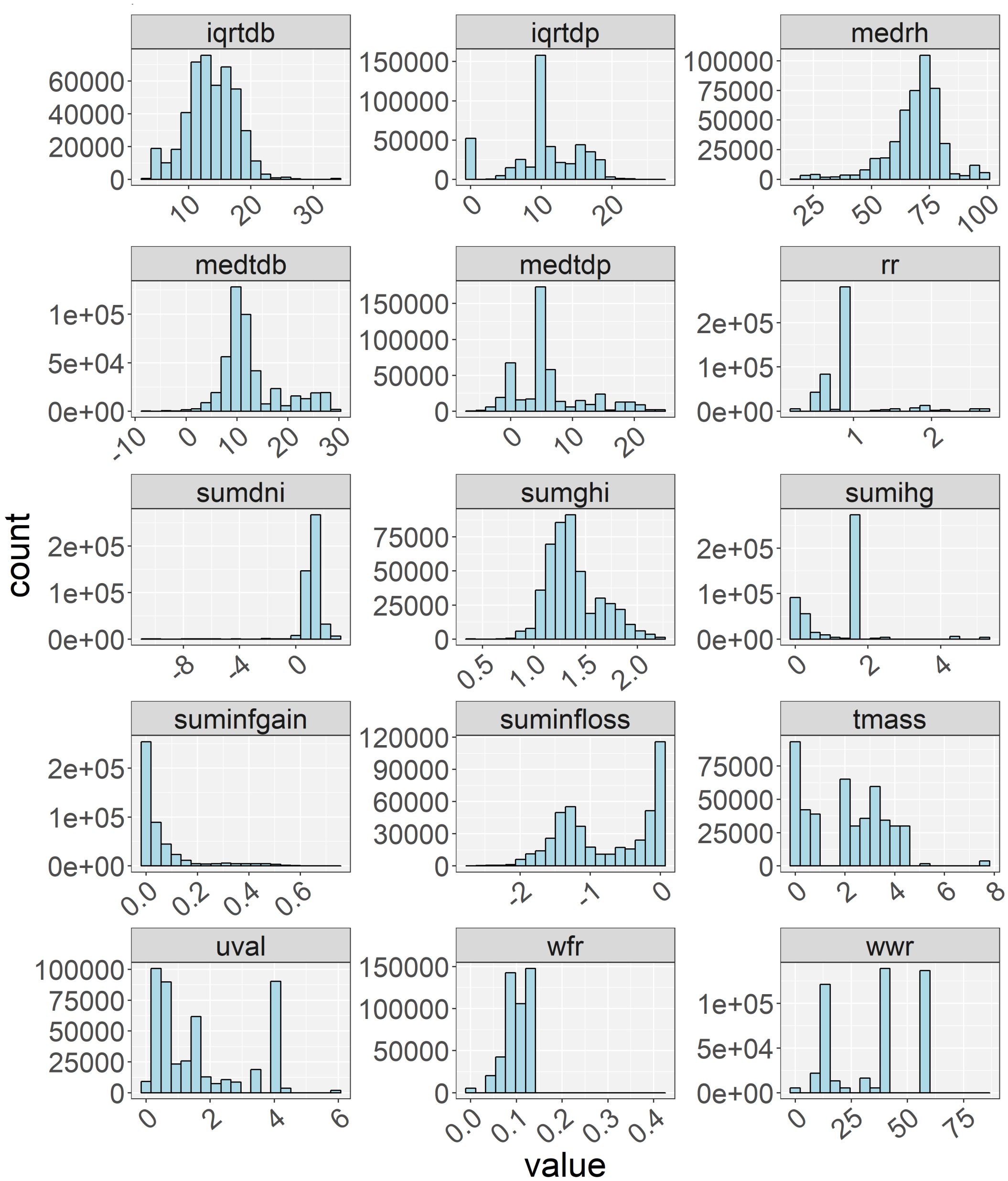


Figure 5: Distribution of features for EnergyPlus data.

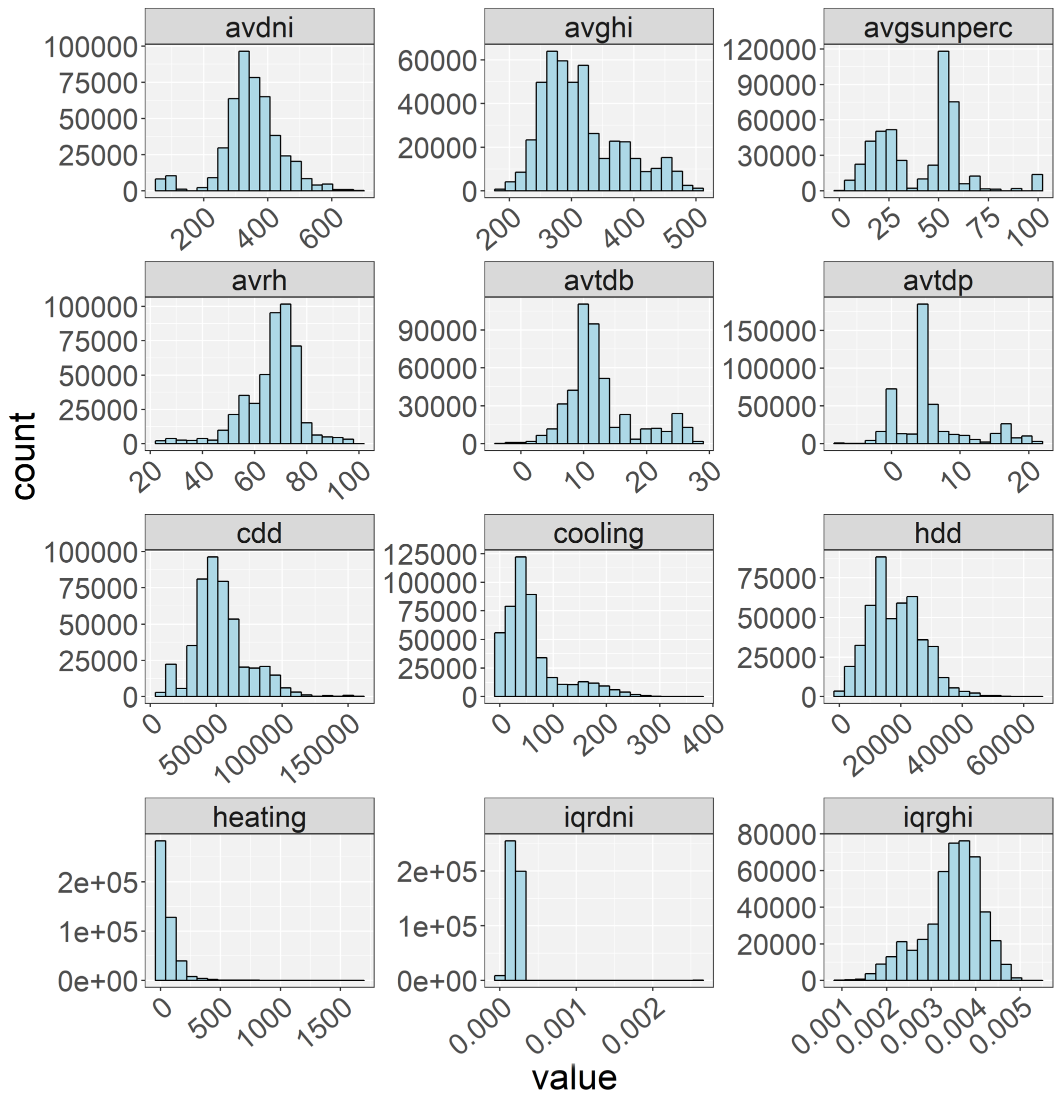


Figure 5 (Cont.): Distribution of features for EnergyPlus data.

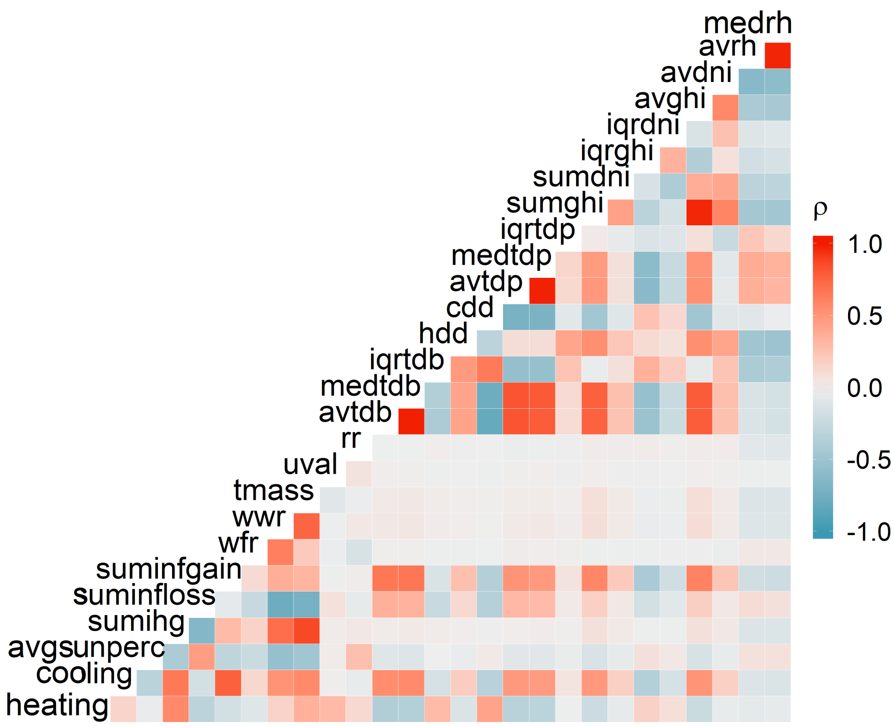


Figure 6: EnergyPlus data features correlation map.

Table 5: Result of tuning ML model for Ecotect simulated dataset.

	SVM		RF		NN		GP		GBRT		XGBoost	
	Heat	Cool	Heat	Cool	Heat	Cool	Heat	Cool	Heat	Cool	Heat	Cool
R^2	0.996	0.972	0.998	0.973	0.997	0968	0.981	0.944	0.999	0.995	0.999	0.998
RMSE	0.475	1.622	0.476	1.585	0.491	1.711	1.381	2.279	0.366	0.677	0.300	0.401
MAE	0.654	1.082	0.332	0.98	0.369	1.120	0.852	1.579	0.254	0.486	0.189	0.294
Fit time (s)	2.19	21.09	0.75	0.73	0.106	0.131	18.86	24.63	0.499	0.655	0.326	0.585
Mean fit time (s)	323.77	177.28	0.72	0.75	1.23	0.99	17.00	18.65	0.20	0.19	0.28	0.28
Test time	0.005	0.005	0.090	0.104	0.001	0.001	0.019	0.018	0.021	0.031	0.045	0.107
Number of parameters	2		3		7		3		7		6	
Total iteration	21		36		3240		30		3456		2160	

and SVM models estimate faster than other, which it makes them appropriate tools for applications requiring large amount of simulations to be performed in limited time. One example is consulting the building retrofit companies with optimised solutions. It can be seen that GP is the slowest and least accurate model among others. As discussed before, the time complexity of GP is $O(N^3)$, and the training speed is not comparable with other ML models when a huge number of samples are involved. For this reason studies applying GP limited training size to tens to few thousands of records (Heo et al., 2012; Zhang et al., 2013; Noh & Rajagopal, 2013; Rastogi et al., 2017; Burkhart et al., 2014; Zhang et al., 2015). However, this model is the best choice to handle uncertain data.

Figures 7 (a) and (b) illustrates predicted values using the attuned GBRT model against their corresponding real heating and cooling loads, respectively. The error distribution of these estimations is depicted in Figure 8.

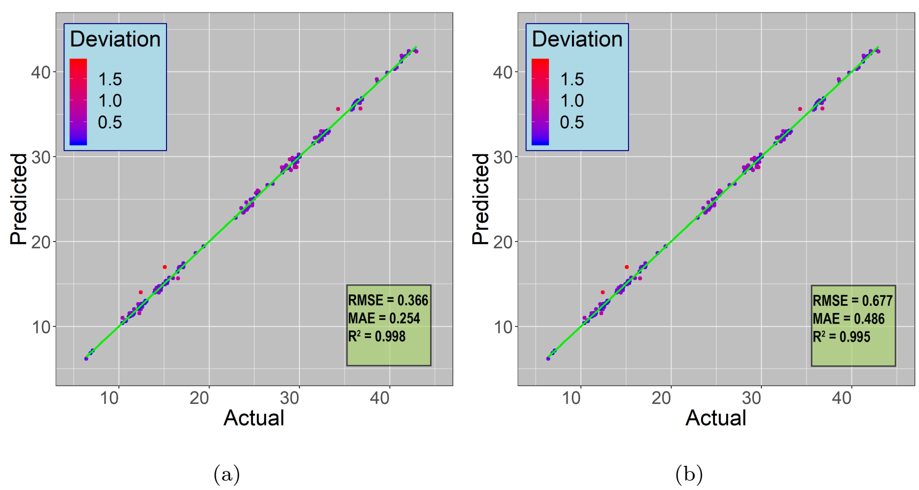
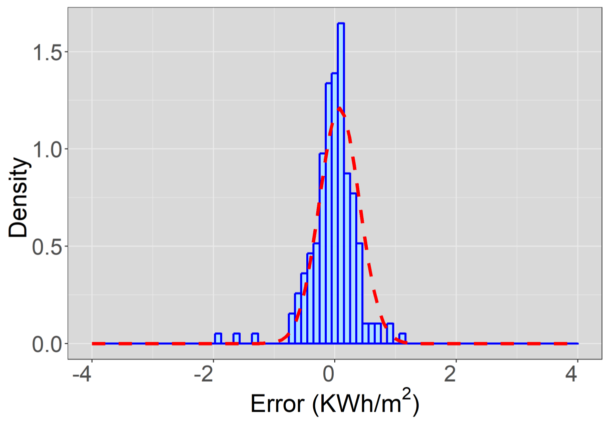
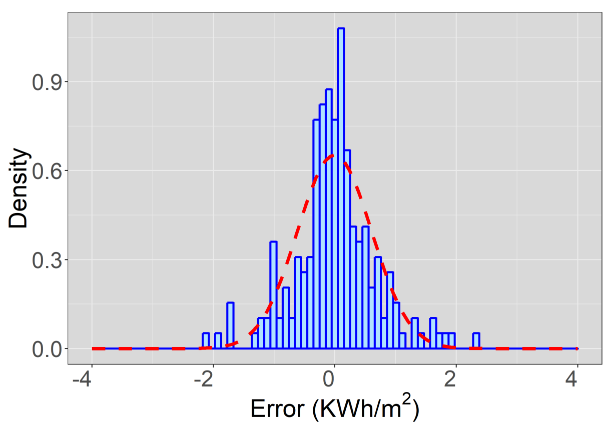


Figure 7: Actual and predicted (a) heating and (b) cooling loads of Ecotect dataset using GBRT model.

For EnergyPlus data, GP is excluded because, as mentioned above, the training time of it is extremely high for large data. The result for rest of the models is presented in Table 6. Here the training size is 4,000 and test is 1,000 where number of folds is 5.



(a)



(b)

Figure 8: Error distribution of (a) heating and (b) cooling loads prediction for Ecotect dataset.

Table 6: Result of tuning ML model for 5000 records of EnergyPlus dataset.

	SVM		RF		NN		GBRT		XGBoost	
	Heat	Cool	Heat	Cool	Heat	Cool	Heat	Cool	Heat	Cool
R^2	0.965	0.973	0.973	0.968	0.966	0969	0.980	0.986	0.982	0.986
RMSE	14.318	8.763	12.720	9.400	14.068	9.376	10.721	6.296	10.386	6.270
MAE	5.622	3.465	5.057	4.841	7.472	4.932	4.400	3.365	4.130	3.143
Fit time (s)	177.66	406.31	6.35	34.873	126.29	10.88	6.363	1.789	4.897	4.871
Mean fit time (s)	1641.91	1197.16	17.6	19.54	21.32	17.19	4.85	4.92	4.61	4.55
Test time	0.483	0.507	0.333	0.595	0.008	0.010	0.244	0.078	0.228	0.219
Number of parameters	2		3		7		3		7	
Total iteration	21		36		3240		3456		2160	

Although all models predict the energy loads with high precision, several factors should be considered to choose the most appropriate one. First, by the increased amount of records, the fitting and forecasting time of SVM significantly rises. The training size of ANN is slightly increased, but still with it is the fastest predictor with a considerable difference with others. GBRT and its advanced model achieve the best RMSE. The original study using GP and a similar number of samples reported mean RMSEs of 23 and 12 kWh/m^2 for heating and cooling loads, respectively (Rastogi et al., 2017), which higher than the ones predicted by other models.

To investigate the effect of data size on the accuracy of supervised models, RMSE is plotted versus the number of train and test records forecasting heating loads of EnergyPlus data which is depicted in Figure 9. Here, a 10 fold cross-validation is used in GBRT model and worst, best and mean RMSE of all folds are presented. Mean training time is also displayed as the top axis for evaluating computational cost. Although the best result is obtained by the highest number of samples, considering the fitting time and error gap, 25,000 record size is enough to build a reliable model. At this point, the mean RMSE is equal to 7.770 kWh/m^2 and required time to fit the model is 66.02 s. Using 400,000 samples and fitting over 2600 s, mean RMSE of 2.338 kWh/m^2 (4% of average heating loads)is achieved.

To demonstrate the performance of GBRT model training and testing over 25,00 of data, the plot predicted heating and cooling values against the actual loads is depicted in Figures 10 (a) and (b). The error distribution of these estimations is depicted in Figure 11.

Most of ML models are capable of forecasting multiple outputs at the same time. However, we tuned all ML regressors separately for heating and cooling loads. None of the techniques obtained the superior accuracies for both target values using the same combination of hyper-parameters. This inconsistency indicates that the importance of input variables as well as the corresponding weights are different. Hence, it is required to fit two independent models rather than training a single model.

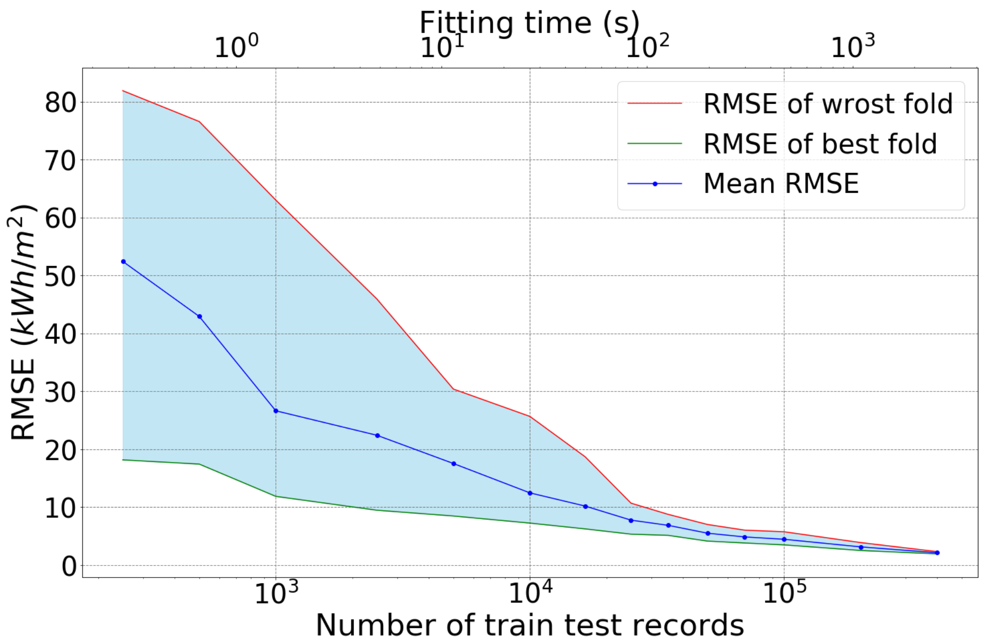
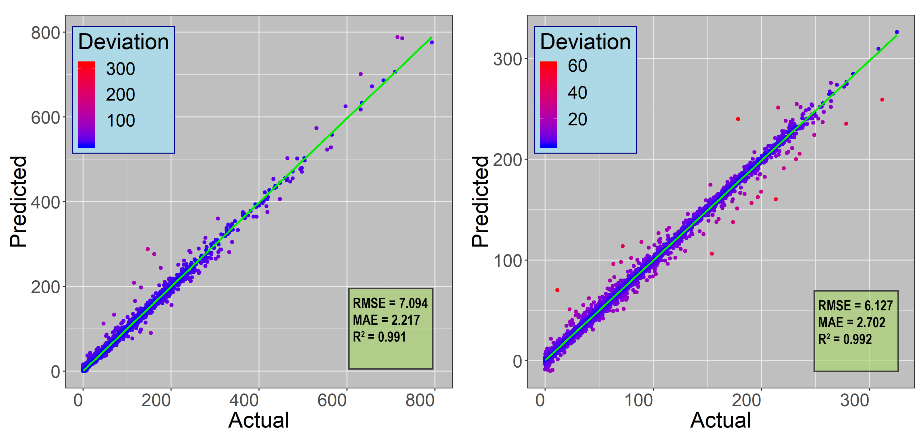
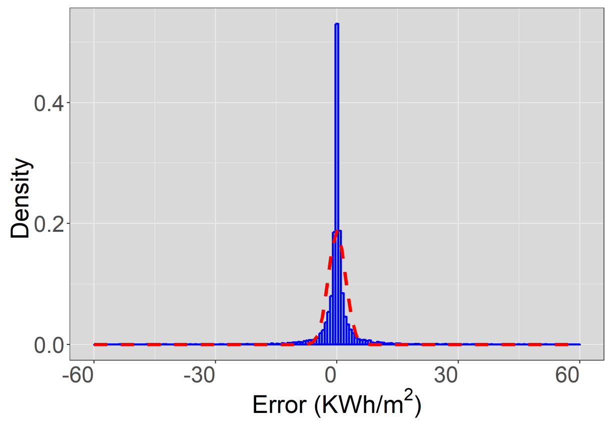


Figure 9: RMSE of heating load prediction against number of total number of train-test samples.



(a) (b)

Figure 10: Actual and predicted (a) heating and (b) cooling loads of EnergyPlus dataset.



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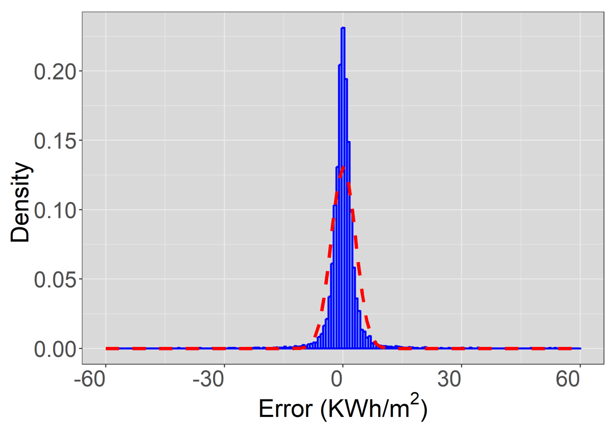


(b)

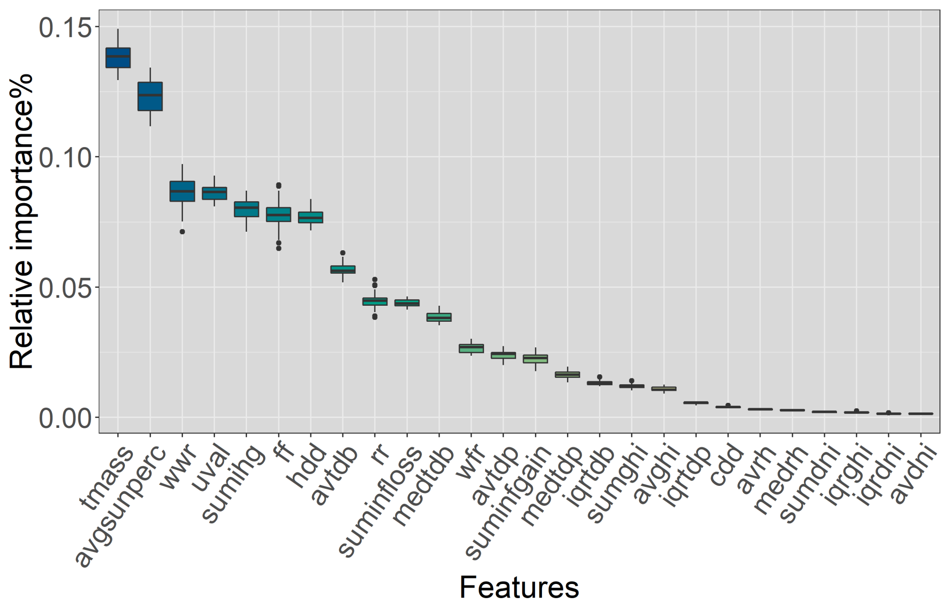
Figure 11: Error distribution of (a) heating and (b) cooling loads prediction for EnergyPlus dataset.

In order to elaborate the importance of features in predicting different loads, sensitivity analysis using two approaches is presented. At first, meta-model based method using RF is utilised. RF creates a lot of decision trees and while training them, the amount of weighted variance decreased by features can be calculated in each tree. For a forest, the variance decline from each feature can be averaged and the features are ranked according to this measure. Here, we trained 30 RF models using 100,000 randomly selected samples to demonstrate the confidence levels of obtained indices. Figures 12 (a) and (b) represents the relative importance of the most principal input variables in forecasting heating and cooling loads.

As the best selected model (i.e. GBRT) doesn't provide the possibility to analyse the sensitivity of the energy model to the input variables, we used a global variance-based method namely Sobol (Sobol, 2001; Saltelli, 2002). Like RF, GBRT does not generate unique trees in every training as there are many factors affecting. Hence, as before we fitted 30 different models and used them to evaluate the 150,000 samples generated by the algorithm. The Sobol first-order indices of features is illustrated in Figure 13. As it can be seen this method is less stable than RF, as the latter one doesn't need an extra distribution of samples, and it is more dependant on the original data used for fitting the model. However, the provided results by Sobol are more generalised.

Although it is not possible to generally rank the feature importance based on the two methods, the input variables with the least impact on the prediction of energy loads can be distinguished. The reason for influential inputs to be ranked differently is that the ML models treat dataset diversely. Even a model with unique hyper-parameters might and fitting the same training data may assign various weights to the features.

The identified features set to drop includes 'avrh', 'avdni', 'iqrdni', 'iqrghi', 'medrh', 'sumdni' for both loads and 'avghi', 'sumghi' additionally for cooling. As it can be seen, all the identified variables are climate related which does not play important role on building energy consumption. It should be noted that all these details are extracted from the dataset and we cannot generalise



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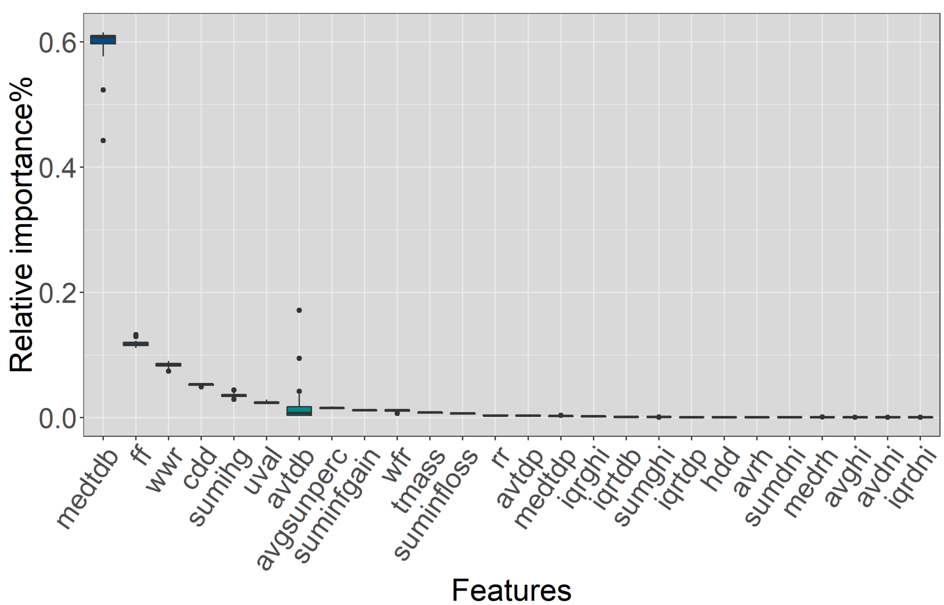
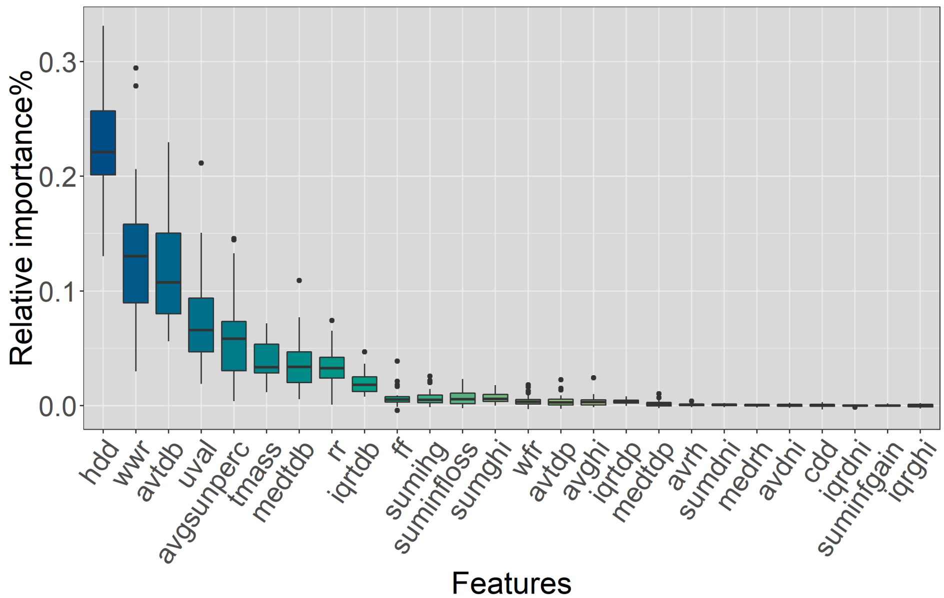


(b)

Figure 12: Importance of features for (a) heating and (b) cooling loads prediction using RF model.



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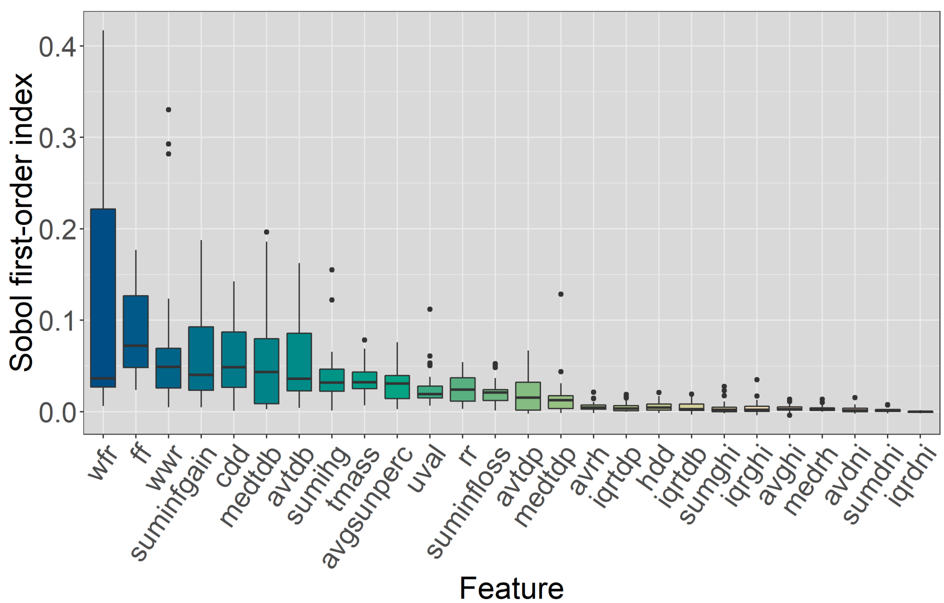


(b)

Figure 13: Sobol first-order indices of features in predicting (a) heating and (b) cooling loads using best ML model.

them to all buildings and even the whole EnergyPlus simulations. There have been several assumptions and limitations in creating the building models and simulations that affect the energy load predictions. Therefore, as we indicated before, the feature extraction and optimisation of machine learning should be based on the application.

Finally, the GBRT with optimal parameters is trained and tested ten times each with 25,000 random samples considering both full and selected feature set. Here, 10-fold cross-validation is used for each model and mean values of RMSE, MAE, R^2 as well as fit and score time of folds are collected. As it can calculated, the elapsed times are related to training of 22500 samples and evaluating 75000 remaining ones. The result of this experiment is summaries in Table 7. It can be seen that there isn't much difference in accuracy of model indicating that unimportant features does not negatively affect the model performance. However, as it was expected the time complexity of training model is reduced due to reduction in dataset dimension.

Table 7: Performance comparison of ML models with full feature set and dropping the inputs determined by sensitivity analysis.

	Heating Load		Cooling Load	
	All inputs	Selected inputs	All inputs	Selected inputs
RMSE	7.871	7.648	4.455	4.384
MAE	2.127	2.085	2.314	2.310
R^2	0.991	0.991	0.993	9.993
Fit time (s)	61.621	48.420	9.387	7.700
Test time (s)	0.642	0.622	0.151	0.145

6. Conclusion

The research presented in this paper addresses the gap in using ML methods for estimating building energy loads through a comprehensive study of common ML models fitting over energy simulation data. As became evident in the reviewed literature, despite the wide usage of MLs in this field, a conclusion on selecting the right model for the energy prediction was not possible. The main reason is that most of the research works has focused on the first eminent part of statistical modelling which is features selection. This paper discussed the importance of ML model optimisation in providing fair comparison of different methods in term of accuracy, simplicity of tuning and training and response times of model. This study optimised the hyper-parameters of each model for both heating and cooling loads to obtain the best precision. It was also indicated that when there are two energy indices as cooling and heating loads to be estimated by model, it is desired to optimise and train separate machines. To that end, the role of ML model in recognising most impacting factor in prediction of building loads. The other key outcome of this research is set of recommendations for quick selection of ML model based on the data and usage.

The results indicated that the standard and advanced GBRTs provide the most accurate predictions, considering the RMSE value. However, when the data was simple (in term of input variables and size), SVM was proven to be the best choice because of simplicity and the speed of calculations. The results also ascertained that for complex data sets, multi-layer NNs are more appropriate when there is a massive demand for ever-more energy simulations. In this case, NN was proven to be capable of estimating incredibly faster than other MLs methods. It should be noted that NN is complicated, and requires an expert to particularly tune it for each studied case; otherwise, NNs could fail quickly.

Comparison of tuned models with previous studies highlighted the importance of determining the hyper-parameters for each data set, and the fact that this can become more crucial by increasing the size and intricacy of the examinations set. By fitting individual models for heating and cooling loads, it was shown that one assorted set of model parameters could not accurately estimate the both values. Therefore, unlike previous studies, it is recommended by this study to train models for each energy load independently. The other approach would be the implementation of a specific sorting algorithm to find the balanced values. As results signified, it is suggested to attain a higher accuracy feeding the machines with more number of instances is essential. It might not be a solution for measured historical data, however further simulation using various values of inputs could be aggregated during design stage prior to optimising the building. Another identified critical factor was that the features must be thoroughly selected/created for representing building characteristics and needs should be properly investigated before developing models.

The findings of this study concurred with the seminal literature by demonstrating the fact that MLs techniques are overtly superior over the conventional statistical and engineering methods in building energy calculation. This study also revealed the further power of those ML methods and newly developed ones when they thoroughly optimised. There are several ready to use software packages (e.g. Matlab) providing various ML models with few parameters to modify. Nevertheless, it is advisable to use simpler models like SVM or RF with an advanced programming language, such as Python and R.

Finally, the most important features are recognised using sensitivity analysis methods, and the investigation of model with reduced dimension revealed that even though the computational cost of building model is reduced, the performance didn't alter. This analysis demonstrated the capability of MLs in eliminating inessential input parameters, while most statistical methods are very sensitive to these type of features.

The methods discussed in this work proved the efficiency of ML models in predicting building energy loads as well as performance. The fast and accurate calculation of those values pave pathways for more informed and productive design decisions for built environments. Furthermore, along with the optimisation algorithms, ML seems as a promising solution for efficacious retrofit planning of complex buildings, where engineers are not capable of massive calculations.

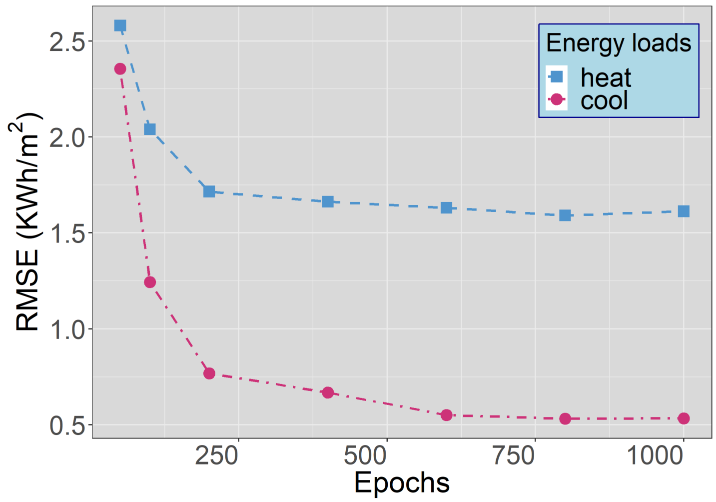
Appendix A. Detailed Results for Tuning ML Models

The detail of tuning each ML model is presented in this section. Some models have several parameters, so the brute force search includes thousands of train-test models. Therefore, it is not possible to present the list of all results in this paper. However,Tables A.8 to A.13 demonstrates the parameters for the best models predicting energy loads of both datasets. In each table the best model is highlighted with light blue colour.

Table A.8: Detail of optimising SVM for both datasets.

EPlus Data		Ecotect Data		SVM Parameters	
Heat RMSE	Cool RMSE	Heat RMSE	Cool RMSE	C	Gamma
14.318	9.785	0.677	1.622	10,000	1
18.988	9.774	0.654	1.667	1000	1
15.720	9.261	0.660	1.756	1,000,000	0.1
15.313	10.302	0.978	1.842	1,000,000	1
21.626	8.763	0.815	2.048	100,000	0.1
31.415	9.452	2.108	2.636	10,000	0.1
43.719	17.833	2.627	3.365	10,000	0.01
60.974	31.658	3.304	3.886	1	0.1
60.974	31.658	3.304	6.550	1	0.01

In order to reduce the time complexity of tuning ANN model, the number of epochs was fixed at 500 and the other parameters were optimised. Then the optimal number of propagations was separately obtained using the best parameters. As shown in the Figures A.14 (a) and (b)



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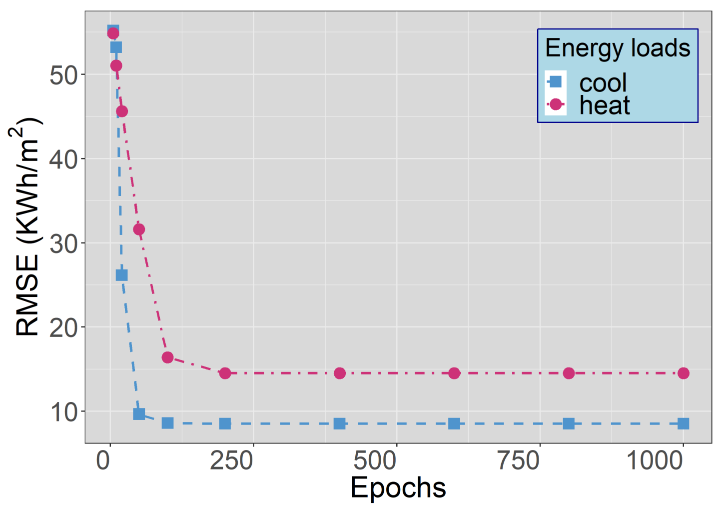

(b)

Figure A.14: RMSE of ANN model predicting energy loads for (a) EPlus and (b) Ecotects datasets against number of epochs.

Table A.9: Detail of optimising RF for both datasets.

EPlus Data		Ecotect Data		RF Parameters		
Heat RMSE	Cool RMSE	Heat RMSE	Cool RMSE	Bootstrap	Max features	No. of estimators
12.873	9.894	0.568	1.585	False	sqrt	600
12.720	9.693	0.576	1.605	False	sqrt	400
14.556	10.734	0.604	1.612	True	sqrt	200
13.334	10.214	0.502	1.658	False	log2	1000
14.551	9.691	0.476	1.683	True	auto	600
14.584	9.600	0.478	1.691	True	auto	800
24.189	13.727	0.536	1.814	False	auto	1000
14.199	10.995	0.616	1.604	True	sqrt	400

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Table A.10: Detail of optimising GBRT for both datasets.

EPlus Data		Ecotect Data		GBRT Parameters						
Heat RMSE	Cool RMSE	Heat RMSE	Cool RMSE	Learning rate	Max depth	max features	Min sample leaf	Min sample split	No. estimator	Sub sample
13.157	7.402	0.388	0.677	0.15	8	None	1	100	1500	1
11.534	6.667	0.366	0.893	0.15	3	None	1	2	1500	1
12.914	6.297	0.399	1.033	0.25	3	sqrt	1	2	1500	1
10.721	8.855	0.514	1.261	0.1	8	sqrt	1	2	2000	1
13.257	9.608	0.523	1.578	0.01	13	sqrt	1	2	1250	0.9
17.843	8.654	3.77	3.895	0.01	8	sqrt	200	100	500	1
22.775	9.856	8.732	8.524	0.001	13	sqrt	200	100	1250	0.7
26.221	15.625	10.054	9.725	0.25	3	sqrt	1000	100	1750	1
35.518	21.196	10.003	9.726	0.1	8	sqrt	1000	1000	1000	0.9
46.991	24.279	9.996	9.720	0.1	3	sqrt	1000	2	1000	0.8
49.515	24.542	9.996	9.722	0.1	3	None	1000	100	1500	0.7
21.578	11.642	10.422	9.746	0.15	13	None	500	1000	1000	0.8

Table A.11: Detail of optimising XGBoost for both datasets.

EPlus Data		Ecotect Data		XGBoost Parameters					
Heat RMSE	Cool RMSE	Heat RMSE	Cool RMSE	Portion of features	Learning rate	Max depth	Min child weight	No. estimator	Sub sample
10.909	8.145	0.303	0.401	0.6	0.1	8	1	1750	0.9
11.616	9.002	0.300	0.452	0.6	0.1	13	1	750	0.7
12.273	8.048	0.323	0.573	0.38	0.1	8	1	1250	0.8
12.436	8.18	0.329	0.804	0.6	0.01	13	1	1750	1
11.302	6.270	0.413	1.131	0.6	0.1	3	1	2000	0.7
10.387	6.382	0.409	1.115	0.6	0.1	3	3	2000	0.9
13.738	9.982	0.306	0.443	0.5	0.1	13	1	1750	0.8
16.030	12.706	0.337	0.557	0.4	0.5	13	3	1000	0.7
20.003	10.434	0.304	0.433	0.1	0.1	8	1	10000	0.8
23.821	14.138	0.343	0.567	0.1	0.25	13	3	1000	0.7
26.266	16.581	0.365	0.578	0.1	0.5	13	3	1500	0.8
57.263	35.554	9.459	10.412	0.6	0.01	3	1	200	0.7

Table A.12: Detail of optimising GP for both datasets.

Ecotect Data		GP Parameters		
Heat RMSE	Cool RMSE	Alpha	Kernel	No. restarts
1.382	2.279	1e-08	Mattern	2
1.381	2.383	1e-12	RBF	4
8.472	2.332	1e-8	RBF	2
8.471	2.333	1e-10	RBF	0
1.383	3.138	1e-4	Mattern	0
4.440	4.238	1e-6	RBF	4

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Table A.13: Detail of optimising ANN for both datasets.

EPlus Data		Ecotect Data		ANN Parameters				
Heat RMSE	Cool RMSE	Heat RMSE	Cool RMSE	Activation	Batch size	No. hidden layers	No. neurons	Optimiser
30.456	12.103	0.492	1.829	Logistic	10	1	2N	lbfgs
30.675	15.847	0.781	1.711	Tanh	10	1	2N	lbfgs
14.631	9.973	0.884	3.389	Tanh	1	2	N, 2N	adam
17.337	9.376	1.052	3.308	Tanh	10	3	3N, 2N, N	lbfgs
14.068	9.754	2.616	3.388	Tanh	1	1	2N	adam
41.157	18.079	4.476	6.645	Relu	1	2	N, 2N	adam
27.573	13.994	10.005	9.73	Logistic	10	3	3N, 2N, N	adam
51.323	26.502	14.453	15.968	Relu	auto	1	N	adam
49.118	25.223	6.401	7.010	Identity	1	2	N, N/2	adam
80.052	57.114	23.506	25.482	Logistic	10	2	3N, N/2	adam

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